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Two energy scales and slow crossover in $YbAl_3$

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Abstract

We present results for $YbAl_3$ which show that the susceptibility, 4f occupation number and the entropy exhibit a slow crossover between the Fermi liquid and local moment regimes. Both the susceptibility and the linear specific heat coefficient exhibit low temperature peaks that imply that in addition to the Kondo scale ($T_K \approx 500$ K) there is a second low temperature scale ($T_{coh} \approx 50$ K) for the onset of coherence. We discuss these results in the context of the Anderson lattice in the limit of low conduction electron density.

Keywords: Intermediate valence; Anderson lattice; Exhaustion

Recent theoretical studies of the Anderson lattice (AL) suggest that as the background conduction electron density n_c decreases the scale T_{coh} for the onset of Fermi liquid coherence becomes significantly smaller than the single impurity Kondo scale T_K [1]. For $T < T_{coh}$ new peaks (in addition to those expected on the scale T_K) are predicted for the susceptibility and specific heat. In addition [2], as n_c decreases, the crossover from low temperature Fermi liquid behavior to high temperature local moment behavior becomes slower than predicted for the Anderson Impurity Model (AIM). This theoretical work was motivated by the desire to understand "Nozieres exhaustion" [3], i.e. how the conduction electrons can screen the 4f spins when the number of conduction electrons n_c is smaller than the number n_f of 4f's in the lattice. Recently we have given evidence [4] for such a slow crossover in the intermediate valence (IV) compounds $YbXCu_4$ (X = Ag, Cd, Mg, Tl, Zn). In this paper we give evidence *both* for a slow crossover *and* for two energy scales in the IV compound $YbAl_3$.

In Fig. 1 we plot the susceptibility $\chi(T)$ and the linear coefficient of the 4f specific heat, where $\gamma_m = C_m/T$ and $C_m = C(YbAl_3) - C(LuAl_3)$. The broad peaks near 100 K are typical of Yb IV compounds with $T_K \sim 500$ K. In addition, there is a peak at 15 K in the susceptibility [5] and a maximum in the specific heat coefficient at $T = 0$. These additional peaks give the basic evidence for the existence of a low temperature scale, $T_{coh} \lesssim 50$ K. Further evidence can be seen in the Hall effect, whose derivative dR_H/dT changes sign at 50 K [6]. As in Ref. [4], we show that the crossover from Fermi liquid behavior to local moment behavior is slower than predicted by the AIM (calculated in the non-crossing approximation) by comparing the data to the AIM result that holds for the measured ground state values of the susceptibility and 4f occupation number n_f. (The latter was measured using Yb L_3 X-ray absorption (XRA).) We fixed the spin–orbit splitting ($\Delta_{so} = 1.3$ eV) and we fixed the width W of the conduction band (assumed Gaussian $N(E) = e^{-E^2/W^2}/\sqrt{\pi}W$) to give the same specific heat coefficient that we observed in $LuAl_3$ ($\gamma = 4$ mJ/mol-K^2). The values of the f-level energy E_f and the 4f/conduction hybridization V that yield the measured $n_f(0)$ and $\chi(0)$ then can be determined uniquely. The values of the parameters are given in

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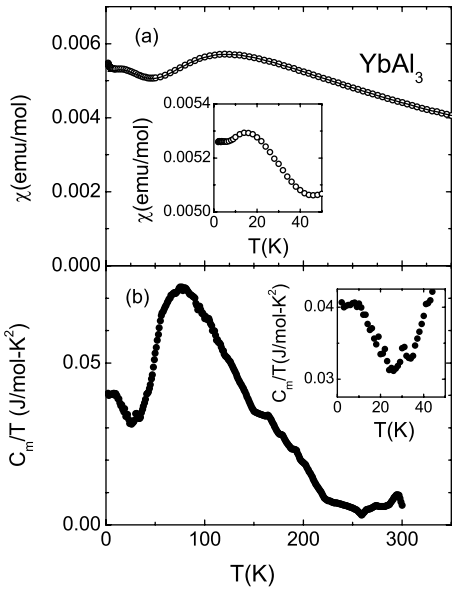

Fig. 1. (a) The magnetic susceptibility $\chi(T)$ and (b) the magnetic contribution to the specific heat coefficient C_m/T for $YbAl_3$. The insets exhibit the low temperature behavior.

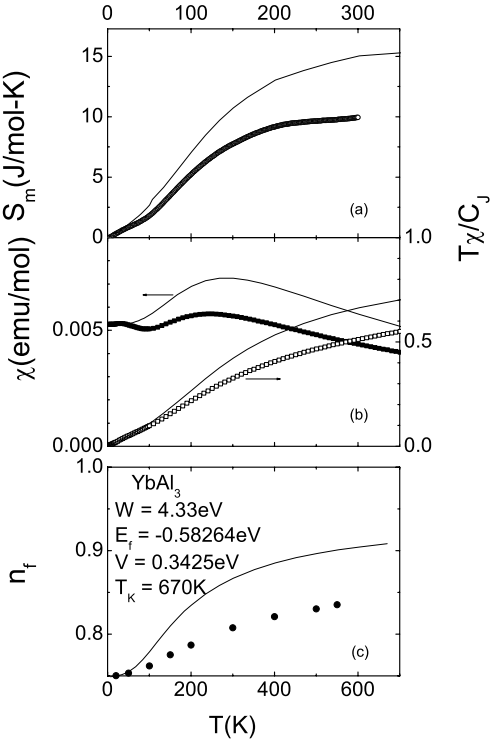

Fig. 2. (a) The 4f entropy S_m, (b) the susceptibility $\chi(T)$ (solid symbols) and the effective moment $T\chi/C_J$ (open symbols) where C_J is the $J = \frac{7}{2}$ Curie constant and (c) the 4f occupation number $n_f(T)$ for $YbAl_3$. The solid lines are the predictions of the Anderson Impurity Model, with input parameters given in the figure.

Fig. 2; T_K is determined from the formula

$$T_K = \left(\frac{V^2}{\sqrt{\pi}W|E_f|}\right)^{1/8}\left(\frac{W}{\Delta_{so}}\right)^{6/8} W e^{\sqrt{\pi}WE_f/8V^2}$$

which includes the effect of spin orbit splitting but ignores crystal field splitting since $T_{cf} \ll T_K$.

Fig. 2 clearly demonstrates that the crossover to local moment behavior is slower than expected based on the Anderson Impurity Model and Fig. 1 demonstrates the existence of a new low temperature scale for $YbAl_3$. For the Anderson lattice, such results are expected [1,2] as the conduction electron density decreases from the value $n_c = 1$ appropriate to a half-filled band when $n_f = 1$. In our recent work [4] on $YbXCu_4$ we assumed a one-band model and deduced n_c from the value of the Hall coefficient for the corresponding Lu compound: $n_c = 1/eR_H(LuXCu_4)$. The slow crossover emerged when the number of electrons per atom (the number per formula unit divided by the number of atoms in the formula unit) decreased below the value unity. Strong deviations occurred for $YbMgCu_4$ where $n_c \sim 0.5$/atom. Using the same approximations for $YbAl_3$ we deduce from the Hall coefficient of $LuAl_3$ [6] that $n_c \sim 0.5$/atom. Hence, while the conduction electron density is not low for $YbAl_3$, it is (in this approximation) as low as in other compounds where strong deviations from the AIM are observed. A number of years ago we gave evidence [7] based on the susceptibility and transport behavior for the existence of two energy scales in the IV compound $CePd_3$. The conduction electron density of $CePd_3$ is less than 0.1 carrier/atom. Hence such results may be generic to IV compounds.

Neutron scattering results [8] for polycrystals of $YbAl_3$ show a Lorentzian excitation centered at $E_0 = 40$ meV. This is as expected for a Anderson impurity: for the parameters of Fig. 2 the AIM predicts $E_0 = 39.6$ meV. In addition, a new excitation centered at 30 meV arises below 50 K, corresponding to the onset of coherence. However, the low temperature form factor [5] is that of a free Yb^{+3} ion, unlike the case of $CePd_3$ where a 5d component sets in below T_{coh}.

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